Hartree-Fock on a superconducting qubit quantum computer

Year: 2020 | Citations: 795 | Authors: F. Arute, K. Arya, R. Babbush, D. Bacon, J. Bardin

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Abstract

Twelve-qubit quantum computing for chemistry Accurate electronic structure calculations are considered one of the most anticipated applications of quantum computing that will revolutionize theoretical chemistry and other related fields. Using the Google Sycamore quantum processor, Google AI Quantum and collaborators performed a variational quantum eigensolver (VQE) simulation of two intermediate-scale chemistry problems: the binding energy of hydrogen chains (as large as H12) and the isomerization mechanism of diazene (see the Perspective by Yuan). The simulations were performed on up to 12 qubits, involving up to 72 two-qubit gates, and show that it is possible to achieve chemical accuracy when VQE is combined with error mitigation strategies. The key building blocks of the proposed VQE algorithm are potentially scalable to larger systems that cannot be simulated classically. Science, this issue p. 1084; see also p. 1054 Accurate quantum simulations of chemistry are performed using up to 12 superconducting qubits and 72 two-qubit gates. The simulation of fermionic systems is among the most anticipated applications of quantum computing. We performed several quantum simulations of chemistry with up to one dozen qubits, including modeling the isomerization mechanism of diazene. We also demonstrated error-mitigation strategies based on N-representability that dramatically improve the effective fidelity of our experiments. Our parameterized ansatz circuits realized the Givens rotation approach to noninteracting fermion evolution, which we variationally optimized to prepare the Hartree-Fock wave function. This ubiquitous algorithmic primitive is classically tractable to simulate yet still generates highly entangled states over the computational basis, which allowed us to assess the performance of our hardware and establish a foundation for scaling up correlated quantum chemistry simulations.